

CONCEPTUAL MODEL TOOLS IN THE PETRASIM GRAPHICAL USER INTERFACE FOR THE TOUGH2 SUITE OF SIMULATORS

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ABSTRACT

PetraSim—an integrated program for model creation, analysis, and results display using the TOUGH2 suite of simulators—has undergone continual development since its first release in August 2002. The latest release (version 5.2) includes a conceptual model Layer Manager which, when used in conjunction with internal boundaries, allows the user to quickly create meshes with varying element shape (rectangular vs. polygonal) thickness, and size. Other new features include: TOUGH2-MP support with automatic execution on multiple core machines; conceptual model wells that can be used to apportion total injection and production rates across elements that intersect the well completion interval; and flux boundary conditions in which the flux rate for individual cells is proportional to the surface area of the element. We will demonstrate these features and discuss the new features being developed for PetraSim version 6.0.

PETRASIM FEATURES

PetraSim provides four key features that help speed and simplify the use of the TOUGH2 family of codes: (1) use of a high level model description based on geometric features of the reservoir, (2) presentation of the required input options grouped in a logical format with appropriate default options activated, (3) automatic writing and execution of the input file, and (4) rapid access to visualization of results. PetraSim is interactive, with immediate visual confirmation of any user actions.

The Conceptual Model

PetraSim allows the user to define layers and regions as high-level geometric entities, independent of the grid. For example, Figure 1 shows a model in which conceptual layers have been defined and can then be used to control material properties, initial conditions, and the spacing of cells in the z direction.

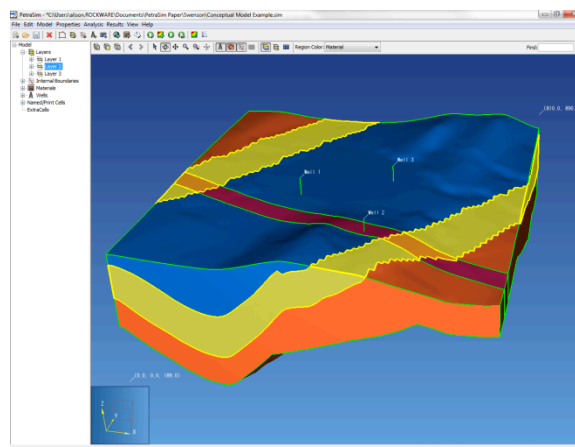


Figure 1. Model with layers and regions defining material boundaries, Layer 2 is highlighted in yellow.

Layers can be broken up into regions using internal boundaries, which are surfaces or planes that typically intersect many layers. Like layers, regions can be used to define material properties and physical and chemical initial conditions. In Figure 1, note that three conceptual layers are intersected by two planar internal boundaries used to represent a crosscutting material change—in this case a fault zone colored red.

Conceptual model layers and regions are independent of the mesh. When the grid is created, the cell properties will inherit the proper material values and initial conditions from the layer or region in which they are located.

Layer boundaries and internal boundaries can be created using xyz ASCII files, DXF files composed of triangular meshes, or through the definition of planar orientation. Conceptual layers are generally used to represent boundaries between stratigraphic formations, while internal boundaries often represent fault zones or other types of structures, but can represent stratigraphic boundaries as well.

Figure 1 also illustrates several options for high-level interaction with the model. On the left of the window is a tree that displays features in the model. Using the tree, the user can select a specific feature. Alternatively, the model can be manipulated in the 3D display and features selected with the mouse. In either case, once a feature is selected, all associated properties can be modified.

Grid Definition

An appropriate grid for an analysis must satisfy several constraints: (1) it must be able to capture the essential features of the reservoir, such as stratigraphic layers with different material properties; (2) it must be sufficiently refined to accurately represent regions of high gradient in the solution; and (3) it must satisfy the requirements of the simulator for proper convergence of the solution. PetraSim supports prismatic (rectangular) 3D grids and non-uniform polygonal (voronoi) meshes.

When creating a rectangular grid (Figure 2), the user can simply specify the number of cells to be used along the x and y edges (along with an optional size factor for geometrically increasing cell sizes) or use input similar to the Meshmaker input for TOUGH2 (Pruess et. al., 1999). To specify the Meshmaker input, the user populates a table that defines the direction, number of repeated cells, and the cell sizes.

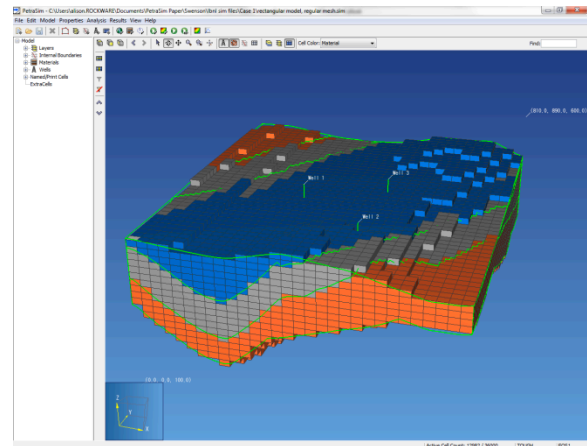


Figure 2. Example of an evenly spaced rectangular grid. Cell color is based on material type.

Input during the creation of a polygonal mesh entails the definition of the maximum cell area, the maximum area of cells adjacent to wells, and the maximum refinement angle, which controls how quickly the cell area near wells disperses to the maximum cell area. Along with providing additional refinement around wells, a polygonal mesh can match an arbitrary model boundary defined during the creation of the conceptual model (Figure 3).

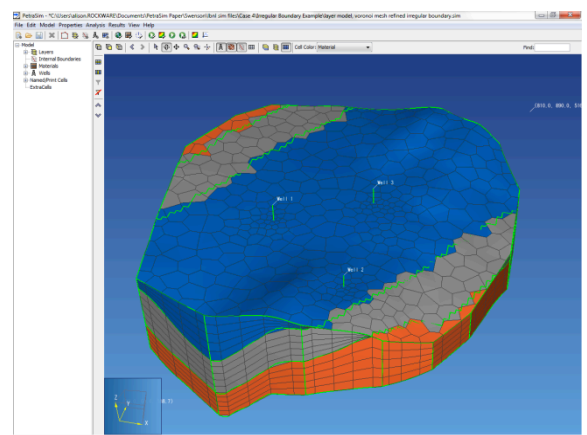


Figure 3. Example of a polygonal mesh that conforms to an irregular model boundary. Cell layer spacing varies with the thickness of the model layer.

Spacing in the z direction is controlled through the Layer Manager. Each model layer is divided into a number of cell layers based on the number of z divisions specified by the user. The thickness of the cell layers vary with the thickness of the model layer (Figure 3). In each

cell column, cell layers can be evenly spaced, or can have variable spacing based on a Dz table. If a Dz table is used, z divisions must be entered such that a fraction of the layer is divided into a specified number of cells.

Editing of Cell Properties

Once a mesh has been created, every cell will be assigned to a region in the conceptual model based on the center of the cell. This allows each cell to inherit the properties of the owning region, such as materials and physical and chemical initial conditions. Cells can be further edited individually or in groups. The user can edit the properties of a cell from the 3D View or Tree View by double-clicking the desired cell, or by selecting the desired cells, right-clicking on one, and selecting Edit Cells... from the context menu. A list of cell IDs and associated material types or PMX values can be imported as an ASCII file to represent complex geology or heterogeneity extracted from more advanced modeling or geostatistical applications.

Model sinks and sources can be added to a single cell or selected group of cells. Input and output rates can be entered in traditional units of kg/s (J/s for heat) or “flux” across the xy area of the cells (kg or J/(s*m²)). This new flux boundary condition allows users to more easily apply a surface boundary condition such as evapotranspiration or recharge to a group of cells with variable volumes. Both traditional and flux-based sinks/sources can be entered as constant values, or can be entered in a time-based table.

Additionally, conceptual model “wells” can be created to represent well completions through multiple adjacent cells (Figure 4). When wells are used, flow in or out of the model can be evenly apportioned across the cells that intersect the completion interval of the well, or the total flow for the well can be proportionally divided based on the product of the permeability and production length within each cell. Like layers and regions, wells are high-level entities that are independent of the grid. Total flow in or out of the well is apportioned to the appropriate model cells when the simulator input file is written.

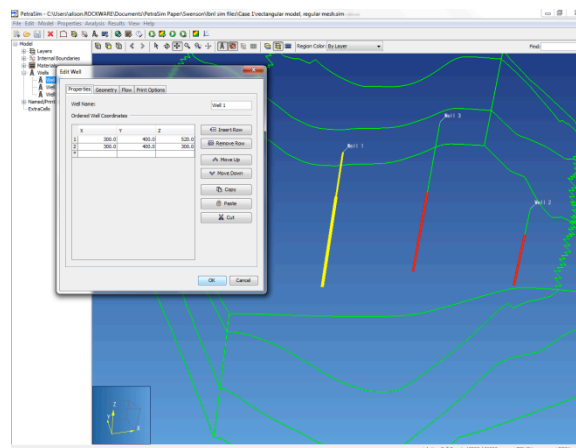


Figure 4. Example of conceptual model wells in PetraSim.

Writing a Simulator Input File

The purpose of a pre-processor is to automatically write the simulator input file in a correct format and without intervention by the user. In PetraSim, this task is performed by a function that accesses the model, the grid, and all other data necessary to write the file.

A portion of an example file is shown in Figure 5. Since the TOUGH2 simulators included with PetraSim have not been modified with respect to input file format, the input file written by PetraSim is in standard TOUGH2 format. Because PetraSim writes the file, there is no need to keep the file small. Each element, connection, and initial condition is written explicitly. It can also be seen that the elements are given sequential numerical names. It is intended that the user never needs to know or examine these names. Any type of data, such as the definition of a source or sink, knows the associated cell and correctly writes the cell name when the simulator input file is written. The resulting input file is correctly formatted and ready for input to TOUGH2.

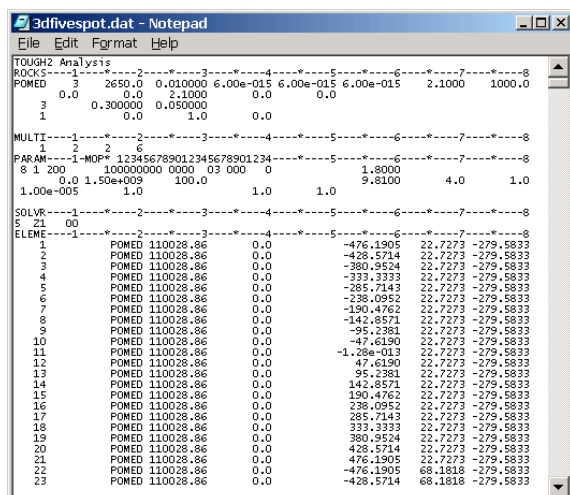


Figure 5. Portion of TOUGH2 input file created by PetraSim

Visualization

After the solution is completed, either 3D or 2D plots of the results can be made. Figure 6 shows an example of an iso-surface plot of temperature. PetraSim uses a common results display component for all simulators. The TOUGH2 simulators included with PetraSim output comma separated value (CSV) files in addition to the normal simulator-specific output. The CSV files provide a consistent format that can be used by both PetraSim and external tools such as MS Excel.

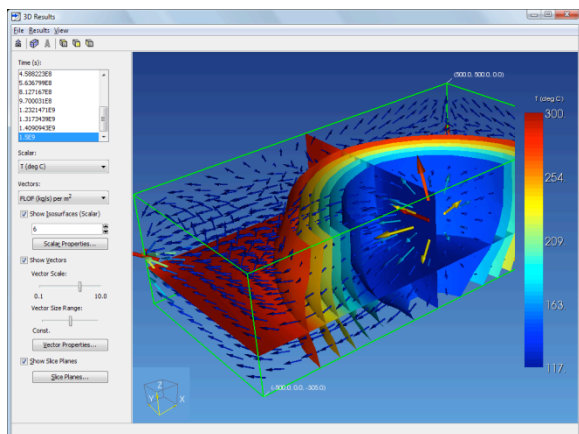


Figure 6. Iso-surface plot of temperatures

As shown in Figure 6, once the data is read, the user can select any available variable and time for plotting. The user can rotate, pan, and zoom the image interactively. Image details, such as the number of iso-surfaces and the data range, can be controlled.

Also, cutting planes can be defined on which the results are contoured. Vectors can be used to display items such as fluid flow. Finally, the user can export the data in a simple X, Y, Z, value format for import into other presentation-quality graphics programs, such as TECPLOT. In PetraSim, results are readily accessible to rapidly evaluate the analysis.

In a similar manner, time history plots and line plots of results can be made. For time history plots, which display results over time for individual cells, data from the FOFT file are used (Pruess, 1999). If FOFT data are not available for a cell, then time series information from the general CSV output files is used. Well plots can be used to show time series data for entire wells (Figure 7). Well plots can show liquid and gas flow rate, as well as the total thermal energy moving in and out of the cells that intersect the completion interval of the well.

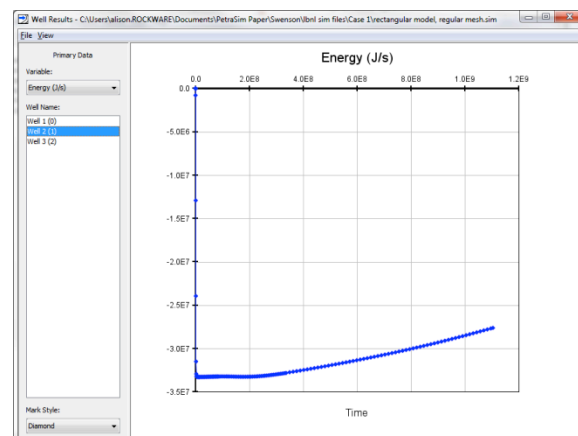


Figure 7. Well Plot showing change in Energy over time.

Line plots are created through the 3D viewer and display an XY plot of a variable along a line. This is useful for viewing the change in a variable, such as temperature or gas saturation along a wellbore over time. Once any plot is made, the data can be exported in a format that can be read in a spreadsheet or other presentation-quality graphics program.

Integrated Solution

Thunderhead Engineering has received a license from the U.S. Department of Energy that allows the integrated distribution of TOUGH2, TMVOC, and TOUGHREACT executables. Therefore, to run the analysis, all the user needs to do is select Analysis->Run TOUGH2 and the analysis will proceed, using the integrated executable. Licensed TOUGH2-MP executables can be purchased with PetraSim and are installed with the software as well.

If the user owns his or her own license for the TOUGH2 source code (can be obtained separately from the US DOE or LBL), PetraSim can be used to write the input file. Then the user can edit the input file to accommodate any specific input changes needed to run their version of TOUGH2.

A QUICK COMPARISON OF LAYERING AND MESH OPTIONS

For comparison purposes, identical material properties, initial conditions and conceptual model wells were applied to four models (Cases 1 through 4). Table 1 describes the various layer and mesh options used in each model.

Table 1. Vertical Division and Mesh Options used in comparison experiment

| Case # | Z Divisions | Mesh Type |
|--------|-------------|-------------|
| 1 | Constant | Rectangular |
| 2 | Constant | Polygonal |
| 3 | Variable | Rectangular |
| 4 | Variable | Polygonal |

Cases 1 and 2 were created with a single conceptual layer (with flat boundaries), and internal boundaries defining the extents of three geological formations (Figure 8). Cells were evenly spaced in the z direction, and cells above and below the top and base of these formations were “disabled” in PetraSim. Cases 3 and 4 were created using three conceptual layers, with the thickness of the model layers varying based on the thickness of the conceptual layers.

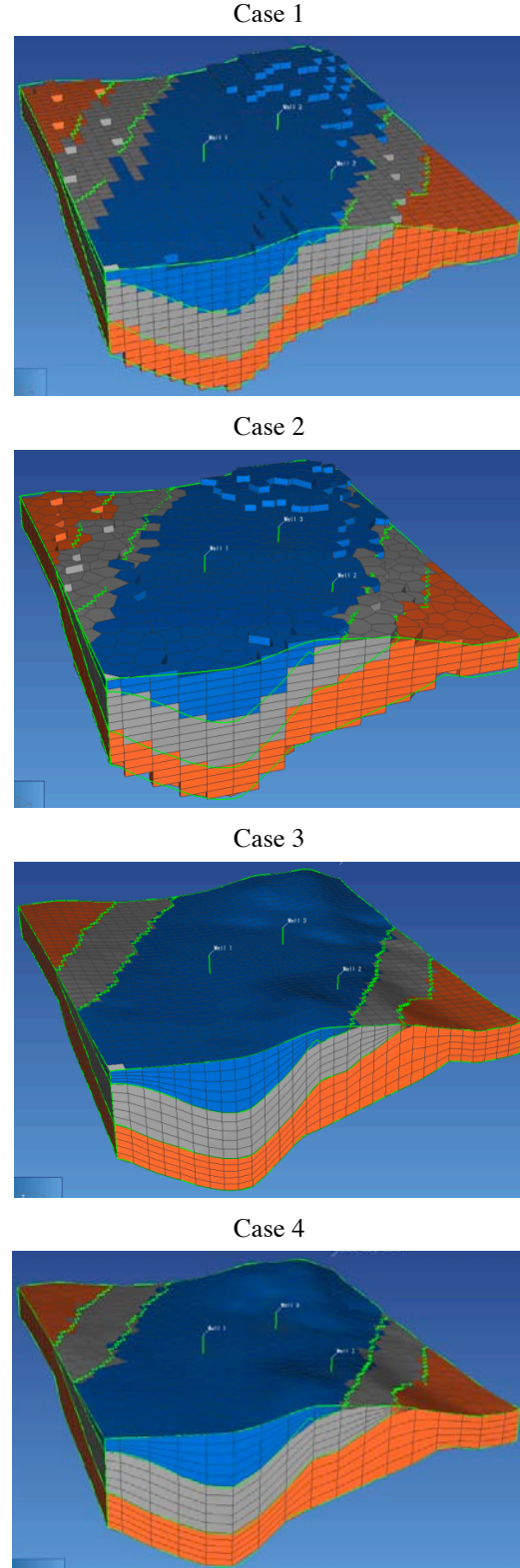


Figure 8. Three-dimensional display of Cases 1 through 4 showing varying mesh and layer geometry

Each model was run to steady-state conditions with closed boundaries to establish linear

pressure and temperature gradients. Results from the steady-state models were loaded as initial conditions into new models to which two production wells (Wells 1 and 2) and one injection well (Well 3) were added. Figure 9 shows the relative locations of Wells 1, 2, and 3.

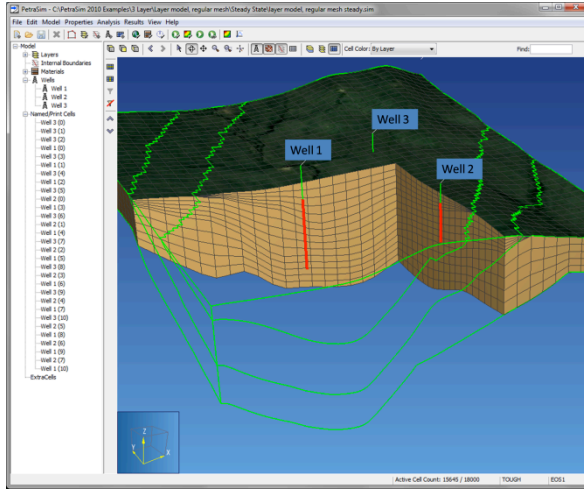
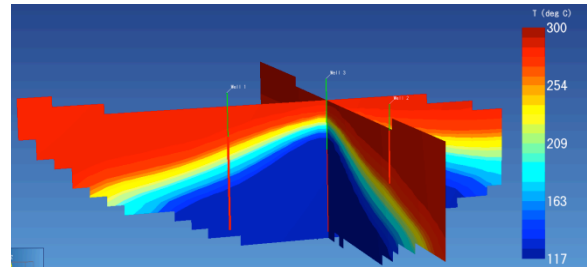


Figure 9. Three-dimensional view of model mesh and labeled well locations

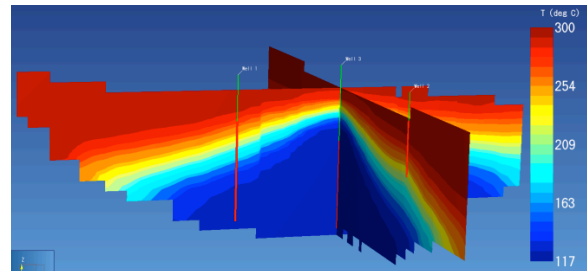
Wells 1 and 2 were production wells using the Well Model option included in TOUGH2. The pressure for each well was determined based on the initial pressure in the center of the top cell that intersected the well completion interval. The productivity index for both wells 1 and 2 was held constant at $2.0\text{E-}12 \text{ m}^3$. Water was injected into Well 3 for 35 years at a constant rate of 30 kg/s and an enthalpy of $5\text{e}5 \text{ J/kg}$. All four models show the same general results at 35 years, with a decrease in temperature from 300°C to around 117°C caused by the injection of colder water at Well 3 (Figure 10).

It should be noted that in order to produce a reasonable temperature distribution in the models with polygonal grids, the area of the elements around the wells needed to be decreased to about $1/6^{\text{th}}$ the area of the cells in the rectangular grids.

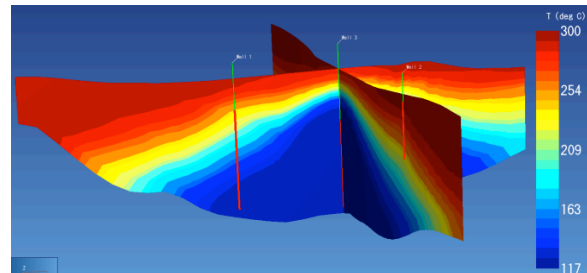
Case 1



Case 2



Case 3



Case 4

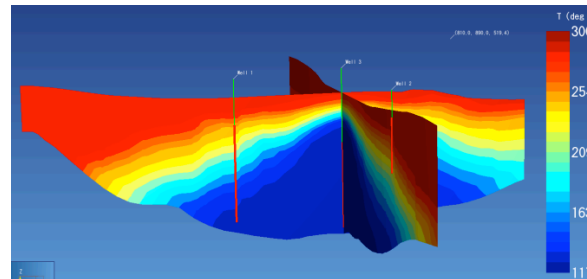


Figure 10. Temperature levels at 35 years in Cases 1 through 4

Even with this increased refinement around wells, the polygonal models had fewer cells and therefore shorter run times than the grid cells with rectangular meshes in the x and y directions (Table 2).

Table 2: Summary of the number of cells, time steps and run times for Cases 1 through 4

| Case # | #Cells | #Time Steps | Run Time (s) |
|--------|--------|-------------|--------------|
| 1 | 12,982 | 160 | 355 |
| 2 | 6,076 | 242 | 255 |
| 3 | 15,645 | 255 | 775 |
| 4 | 7,100 | 248 | 329 |

Well plots showing Energy Production and Flow are similar, although not identical (Figure 11).

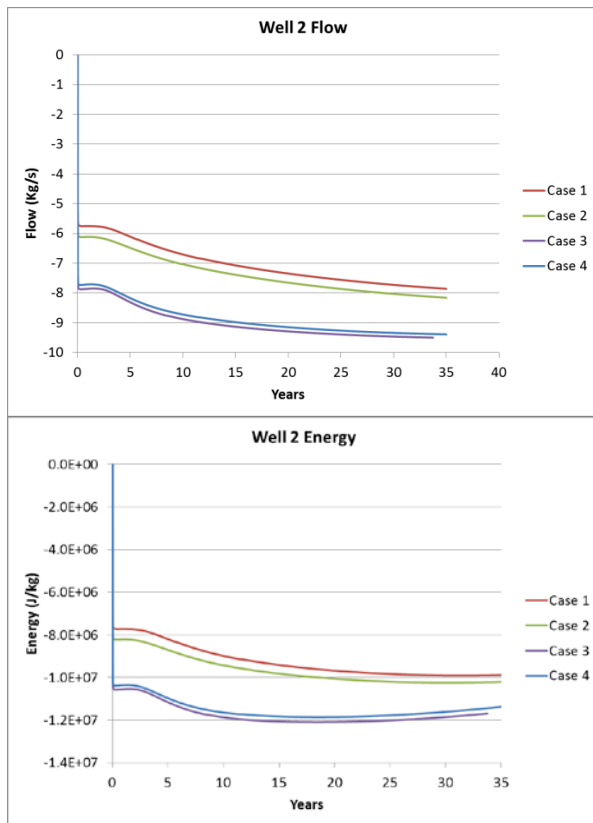


Figure 11. Plots showing Flow and Energy for Well 2 for Cases 1 through 4

Even if the mesh were refined, the type of mesh (i.e., rectangular vs. polygonal) did not affect the flow in and out of the wells. Instead, Well Plot results are grouped based on the use of conceptual model layers. In cases 1 and 2 (uniform horizontal mesh), the flow from Well 1 is greater than cases 3 and 4 (layered mesh in the z direction). Correspondingly, the flow from Well 2 is smaller for cases 1 and 2 and larger for cases 3 and 4. This means that in cases 1 and 2 (with a horizontal Z mesh), it is relatively easier

to flow from Well 3 to Well 1 than from Well 3 to Well 2. The converse is true for the layered models (Cases 3 and 4).

As described by Pruess (1991), for a regular rectangular grid, flow can be preferentially oriented along the rectangular directions and more difficult in the diagonal direction. As shown in Figure 12, flow from Well 3 to Well 2 must cross grid diagonals for cases 1 and 2 (uniform horizontal mesh), while the layered mesh does not require as much flow across the diagonals. It is hypothesized that this is the primary reason that Well 2 produces less flow for cases 1 and 2 and more flow in cases 3 and 4.

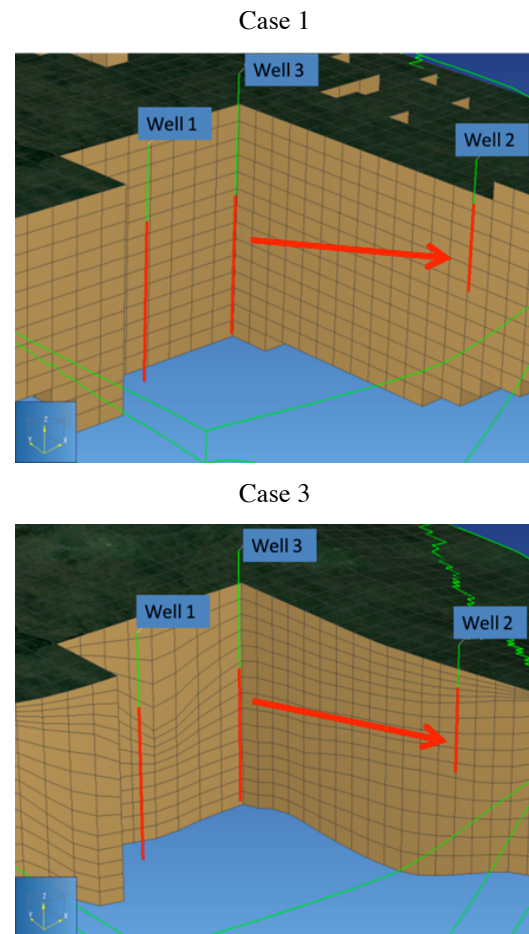


Figure 12. Views showing varying mesh geometry in the z direction for Cases 1 and 3. Red arrows illustrate the intersection of flow vectors from Well 3 to Well 1 with mesh lines.

FEATURES TO BE INCLUDED IN VERSION 6

Development has begun on version 6 of PetraSim. Some of the features to be included are:

- Support for newer TOUGH2 EOS modules, including EO7C and ECO2M
- Support for TOUGH2 v2.1 and TOUGHREACT v2
- Improved support for larger MINC
- Support for the porosity modifier
- Support for more units during model input and result visualization
- More efficient tools for the creation of multiple wells and internal boundaries

OBTAINING PETRASIM

A 30-day trial version of PetraSim can be downloaded at www.petrasim.com. Sales are through RockWare (www.rockware.com). Licenses are available for education (free), research, and commercial use.

ACKNOWLEDGEMENTS

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- Pruess, K., Grid Orientation Effects in the Simulation of Cold Water Injection into Depleted Vapor Zones, Proceedings, Sixteenth Workshop on Geothermal Reservoir Engineering, Stanford University, Stanford, California, , SGP-TR-134, January 23-25, 1991.
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